

Superadiabatic optimization via Dykhne-Davis-Pechukas (DDP) method

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This paper we propose how to apply the Dykhne-Davis-Pechukas (DDP) method for optimization of adiabatic passage in a two-state system in the second adiabatic basis.

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I. INTRODUCTION

In this paper we propose how to utilize a recent idea of Guerin *et al.* [7] who applied the well-known Dykhne-Davis-Pechukas (DDP) method [8] for optimization of adiabatic passage in a two-state system. In order to adapt this approach to STIRAP, we reduce the three-level Raman system to effective two-state systems in two limits: on exact resonance and for large single-photon detuning. The optimization, which minimizes the non-adiabatic transitions and maximizes the fidelity, leads to a particular relation between the pulse shapes of the driving pump and Stokes fields.

II. OPTIMIZATION OF ADIABATIC PASSAGE BETWEEN TWO STATES

The probability amplitudes in a two-state system $\mathbf{c}(t) = [c_1(t), c_2(t)]^T$ satisfy the Schrödinger equation,

$$i\hbar \frac{d}{dt} \mathbf{c}(t) = \mathbf{H}(t) \mathbf{c}(t), \quad (1)$$

where the Hamiltonian in the rotating-wave approximation (RWA) reads [9]

$$\mathbf{H}(t) = \frac{1}{2}\hbar \begin{bmatrix} -\Delta(t) & \Omega(t) \\ \Omega(t) & \Delta(t) \end{bmatrix}. \quad (2)$$

The detuning $\Delta = \omega_0 - \omega$ is the difference between the transition frequency ω_0 and the carrier laser frequency ω . The time-varying Rabi frequency $\Omega(t) = |dE(t)|/\hbar$ describes the laser-atom interaction, where d is the electric dipole moment for the $\psi_1 \leftrightarrow \psi_2$ transition and $E(t)$ is the laser electric field envelope.

A. Adiabatic basis

For the derivation of the transition probability we shall need the adiabatic basis, i.e. the basis of the eigenstates of the Hamiltonian (6). We summarize below the basic definitions and properties of this basis.

The probability amplitudes in the diabatic and adiabatic bases are connected via the rotation matrix

$$\mathbf{R}(\vartheta) = \begin{bmatrix} \cos \vartheta & \sin \vartheta \\ -\sin \vartheta & \cos \vartheta \end{bmatrix}, \quad (3)$$

as

$$\mathbf{c}(t) = \mathbf{R}(\vartheta(t)) \mathbf{a}(t), \quad (4)$$

where the column-vector $\mathbf{a}(t) = [a_-(t), a_+(t)]^T$ comprises the probability amplitudes of the adiabatic states $|\varphi_-(t)\rangle$ and $|\varphi_+(t)\rangle$. These amplitudes satisfy the transformed Schrödinger equation,

$$i\hbar \frac{d}{dt} \mathbf{a}(t) = \mathbf{H}_a(t) \mathbf{a}(t), \quad (5)$$

where the transformed Hamiltonian is given by

$$\begin{aligned} \mathbf{H}_a(t) &= \mathbf{R}^{-1}(\vartheta(t)) \mathbf{H}(t) \mathbf{R}(\vartheta(t)) - i\hbar \mathbf{R}^{-1}(\vartheta(t)) \dot{\mathbf{R}}(\vartheta(t)) \\ &= \hbar \begin{bmatrix} \mathcal{E}_-(t) & -i\dot{\vartheta}(t) \\ i\dot{\vartheta}(t) & \mathcal{E}_+(t) \end{bmatrix}, \end{aligned} \quad (6)$$

where the overdots denote time derivatives. For the reader convenience we write the expression for the non-adiabatic coupling $\dot{\vartheta}(t)$ in terms of $\Omega(t)$ and $\Delta(t)$. Using the definition given by Eq.(9) easily can be seen that

$$\dot{\vartheta}(t) = \frac{\dot{\Omega}(t)\Delta(t) - \dot{\Delta}(t)\Omega(t)}{\Omega^2(t) + \Delta^2(t)} \quad (8)$$

In terms of the mixing angle $\vartheta(t)$, defined as

$$\tan 2\vartheta(t) = \frac{\Omega(t)}{\Delta(t)}, \quad (0 \leq \vartheta(t) \leq \frac{\pi}{2}), \quad (9)$$

the eigenstates of $\mathbf{H}(t)$ read

$$|\varphi_-(t)\rangle = \cos \vartheta(t) |\psi_1\rangle - \sin \vartheta(t) |\psi_2\rangle, \quad (10a)$$

$$|\varphi_+(t)\rangle = \sin \vartheta(t) |\psi_1\rangle + \cos \vartheta(t) |\psi_2\rangle. \quad (10b)$$

The time dependences of the adiabatic states $|\varphi_-(t)\rangle$ and $|\varphi_+(t)\rangle$ derive from the mixing angle $\vartheta(t)$, whereas the bare (diabatic) states $|\psi_1\rangle$ and $|\psi_2\rangle$ are stationary. The energies of the adiabatic states are the eigenvalues of $\mathbf{H}(t)$,

$$\hbar \mathcal{E}_{\pm}(t) = \frac{\hbar}{2} \left[\Delta \pm \sqrt{\Omega^2(t) + \Delta^2} \right]. \quad (11)$$

The splitting between them is given by

$$\hbar \mathcal{E}(t) = \hbar \mathcal{E}_+(t) - \hbar \mathcal{E}_-(t) = \hbar \sqrt{\Omega^2(t) + \Delta^2}. \quad (12)$$

Hereafter we will consider level crossing models. Because the Rabi frequency $\Omega(t)$ vanishes at large times, $\Omega(\pm\infty) = 0$, and because the detuning $\Delta(t)$ sweeps from minus to plus infinity, $\hbar\Delta(\pm\infty) = \pm\infty$, the mixing angle $\vartheta(t)$ rotates clockwise from $\vartheta(-\infty) = \pi/2$ to $\vartheta(+\infty) = 0$, and the composition of the adiabatic states changes accordingly. Asymptotically, each adiabatic state becomes uniquely identified with a single diabatic state,

$$-|\psi_2\rangle \xrightarrow[-\infty]{+\infty} |\varphi_-(t)\rangle \xrightarrow{+\infty} |\psi_1\rangle, \quad (13a)$$

$$|\psi_1\rangle \xrightarrow[-\infty]{+\infty} |\varphi_+(t)\rangle \xrightarrow{+\infty} |\psi_2\rangle. \quad (13b)$$

Because of the level crossing each adiabatic state connects *different* bare states at $-\infty$ and $+\infty$. In the adiabatic limit, the system starts in state $|\psi_1\rangle$ and follows the adiabatic state $|\varphi_+(t)\rangle$ to end up in state $|\psi_2\rangle$. Hence adiabatic evolution and level crossing lead to complete population transfer.

It is important to note that the probability of transition in the adiabatic basis \mathcal{P} is equal to the probability of no transition in the diabatic basis,

$$P = 1 - \mathcal{P}. \quad (14)$$

We will continue with the description of the Dykhne-Davis-Pechukas (DDP) method, which gives the adiabatic probability \mathcal{P} , and we shall use Eq. (14) to find the diabatic probability P .

B. Dykhne-Davis-Pechukas (DDP) approximation

1. A single transition point

A useful and very accurate technique for obtaining the final transition probabilities is the Dykhne-Davis-Pechukas method, or DDP method, first introduced by Dykhne and given a rigorous mathematical formulation later by Davis and Pechukas [8]. The basic idea of the DDP method is that, in the adiabatic limit, the two-state coupling is universal, independent of a given model, and the contributions to the transition probability P between the adiabatic states are given by the complex plane zeros of the adiabatic eigenenergies, in the form of an exponential. Dykhne-Davis-Pechukas (DDP) approximation, [8], which provides the asymptotically exact transition probability P can be also used to estimate the non-adiabatic effects [7]. The DDP formula reads

$$P \approx e^{-2\text{Im}D(t_0)}, \quad (15)$$

where

$$D(t_0) = \int_0^{t_0} E(t) dt \quad (16)$$

is an integral over the eigenenergy splitting $E(t)$. The point t_0 is called the transition point and it is defined as the (complex) zero of the quasienergy splitting,

$$E(t_0) = 0, \quad (17)$$

which lies in the upper half of the complex t -plane (i.e., with $\text{Im} t_0 > 0$). Equation (15) gives the correct asymptotic probability for nonadiabatic transitions provided: (i) the quasienergy splitting $E(t)$ does not vanish for real t , including at $\pm\infty$; (ii) $E(t)$ is analytic and single-valued at least throughout a region of the complex t -plane that includes the region from the real axis to the transition point t_0 ; (iii) the transition point t_0 is well separated from the other quasienergy zero points (if any) and from possible singularities; (iv) there exists a level (or Stokes) line defined by

$$\text{Im}D(t) = \text{Im}D(t_0), \quad (18)$$

which extends from $-\infty$ to $+\infty$ and passes through t_0 .

As has been pointed out already by Davis and Pechukas [8], for the Landau-Zener model, which possesses a single transition point, the DDP formula (15) gives the exact transition probability, not only in the adiabatic limit but also in the general case. This amazing feature indicates the relevance of the DDP approximation.

2. Multiple transition points

In the case of more than one zero points in the upper t -plane, Davis and Pechukas [8] have suggested, that Eq. (15) can be generalized to include the contributions from all these N zero points t_k in a coherent sum. This suggestion has been later verified [? ? ?]. The generalized DDP formula has the form

$$P \approx \left| \sum_{k=1}^N \Gamma_k e^{iD(t_k)} \right|^2, \quad (19)$$

where the Γ_k factors are defined by

$$\Gamma_k = 4i \lim_{t \rightarrow t_k} (t - t_k) \dot{\vartheta}(t). \quad (20)$$

and they usually take values $+1$ or -1 . Here $\dot{\vartheta}(t)$ accounts for the nonadiabatic coupling between the adiabatic states, with $\vartheta(t) = \frac{1}{2} \tan^{-1} \Omega(t)/\Delta(t)$.

In principle, Eq. (19) should be used when there are more than one zero points lying on the lowest Stokes line (the closest one to the real axis) and should include only the contributions from these zeroes. The contributions from the farther zeroes are exponentially small compared to the dominant ones and may therefore be neglected.

C. Adiabatic optimization for two-state system based on the DDP method

It is shown in [7] that Dykhne-Davis-Pechukas (DDP) method [8] can be used to examine the adiabatic limit of population transfer in two-level models driven by a chirped laser field. In [7] the final population transfer

for different trajectories in the parameter space in the adiabatic limit is analyzed.

After using the scaled time $t = \tau/\alpha$, where the parameter $1/\alpha$ under the limit $\alpha \rightarrow \infty$ can be viewed as adiabatic limit, we can write the new scaled Schrodinger equation Eq.(??) for the two-state system. In Eq.(2), we can parameterize the trajectories defined from $\Omega(t)$ and $\Delta(t)$ as a function of time, by assuming a given smooth pulse shape function $0 < \Lambda(t) < 1$, which has its maximum for $t = 0$. This pulse shape function is related to the coupling by

$$\Omega(t) = \Omega_0 \Lambda(t) \quad (21)$$

where Ω_0 is the two-state peak Rabi frequency. In reason to have the constant eigenenergy splitting $E(t)$, accordingly to Eq.(21) the detuning is defined by

$$\Delta(t) = \Delta_0 \text{sign}(t) \sqrt{1 - \Lambda^2(t)} \quad (22)$$

The parametrization given by Eq.(21) and Eq.(22) implies

$$E(t) = \sqrt{(\Delta_0)^2 + [(\Omega_0)^2 - (\Delta_0)^2] \Lambda^2(t)} \quad (23)$$

Using the DDP method, Eq.(17) and Eq.(23) give

$$\Lambda(t_0) = \pm i \frac{\Delta_0}{\sqrt{(\Omega_0)^2 - (\Delta_0)^2}}, \text{ for } \Omega_0 > \Delta_0 \quad (24)$$

$$\Lambda(t_0) = \pm \frac{\Delta_0}{\sqrt{(\Delta_0)^2 - (\Omega_0)^2}}, \text{ for } \Omega_0 < \Delta_0$$

For particular class of analytic functions, defined with $\Lambda(t)$, the following condition is fulfilled

$$\lim_{\text{Im} t_0 \rightarrow \infty} \Lambda(t_0) \rightarrow \infty$$

Using Eq.(24) for this class of models defined with $\Lambda(t)$, the difference between Ω_0 and Δ_0 to tends to zero

$$|\Omega_0 - \Delta_0| \rightarrow 0,$$

is necessary and sufficient condition the imaginary part of the transition points to tends to infinity

$$\text{Im} t_0 \rightarrow \infty.$$

From Eq.(34) can be seen that

$$\lim_{|\Omega_0 - \Delta_0| \rightarrow 0} \text{Im} D(t_0) = \text{Im} \int_0^\infty \Delta_0 dt \rightarrow \infty \quad (25)$$

Therefore, from Eq.(15) follows that the dominant nonadiabatic correction given by the DDP formula vanishes for the level lines defined by Eq.(21), Eq.(22) and $\Omega_0 = \Delta_0$. As have been pointed in [7] in the adiabatic regime, the optimum level lines can be seen as a boundary between decreasing and oscillating regimes for the nonadiabatic correction.

III. SECOND DDP ESTIMATION FOR THE OPTIMIZED ADIABATIC PASSAGE

As we have expalined, Guérin *et al.* [7] have used the DDP method to optimize the adiabatic passage between two states, assuming that the probability for nonadiabatic losses could be determined by the brhaviour of the transition points t_k .

They have proposed to suppress the nonadiabatic losses altogether by choosing the Rabi frequency $\Omega(t)$ and the detuning $\Delta(t)$ such that there are *no transition points*. This condition is obviously fulfilled if the quasienergy splitting is *constant*,

$$\varepsilon(t) = \sqrt{\Omega(t)^2 + \Delta(t)^2} = \text{const.} \quad (26)$$

The later condition also manifests the choice of a detuning and Rabi frequency defined with Eqs. (22) and (21). Easely can be seen that the same detuning and Rabi frequency functions could be parameterized as

$$\Delta(t) = \Omega_0 \sin \left[\frac{\pi}{2} f(t) \right], \quad \Omega(t) = \Omega_0 \cos \left[\frac{\pi}{2} f(t) \right], \quad (27a)$$

$$-1 = f(-\infty) \leq f(t) \leq f(\infty) = 1, \quad (27b)$$

with $f(t)$ being an arbitrary monotonically increasing function with the above property. According to the DDP method such models do not have transition points and lead to vanishing nonadiabatic corrections. The optimization based on DDP is not exact in the sense that it is performed by using approximate technique. It is interesting to calculate the corrections to this DDP optimization. Although we are able to design models that yield according to the DDP, vanishing nonadiabatic corrections there is no way to calculate the transition probability for these models again using DDP method in the diabatic basis. DDP approximation comprise nonadiabatic corrections not only from the first-order perturbation theory in the adiabatic basis but adding the contributions from all orders via correct prefactor. Even so, using DDP not in the diabatic but in the first adiabatic basis is instructive. This is also a way to calculate the deviation form the DDP optimization and to reveal the nature of the oscillation behavior for the transition probability for models that are designed to minimize the nonadiabatic corrections [7]. We note that the the probability of transition in the adiabatic basis \mathcal{P} is equal to the probability of no transition in the diabatic basis and the both are related via (14). Using the parametrization (27a) for the

Schrödinger equation in the adiabatic basis, the transformed Hamiltonian up to phase transformation is given by

$$H_a(t) = \hbar \begin{bmatrix} \Omega_0 & \dot{f}(t) \\ \dot{f}(t) & -\Omega_0 \end{bmatrix}, \quad (28)$$

where the nonadiabatic coupling is given by (8). Nonetheless a particular level crossing model does not have a transition points in the diabatic basis, in the first adiabatic basis, such a model depending on the function $f(t)$ would have transition points. This means that applying a DDP method in the first adiabatic basis instead of the diabatic one, one could analyze the nonadiabatic corrections of the optimized adiabatic passage.

A. Gaussian model

As a particular example we will consider a level crossing model,

$$\Delta(t) = \Omega_0 \sin \left[\frac{\pi}{2} \text{erf}(t/T) \right], \quad \Omega(t) = \Omega_0 \cos \left[\frac{\pi}{2} \text{erf}(t/T) \right]. \quad (29)$$

This model in the adiabatic basis is related to the Gaussian model, which is seen from the Hamiltonian (28).

$$i\hbar \frac{d}{dt} \mathbf{a}(t) = \hbar \begin{bmatrix} \Omega_0 & \frac{\sqrt{\pi}}{T} \exp \left[-(t/T)^2 \right] \\ \frac{\sqrt{\pi}}{T} \exp \left[-(t/T)^2 \right] & -\Omega_0 \end{bmatrix} \mathbf{a}(t),$$

The analytic estimation of the transition probability for the Gaussian model could be performed using DDP. We will briefly review details of such calculation, but the reader could find a similar calculation in more details in [?].

1. Transition points

For the Gaussian model (??), there are infinitely many transition points in the upper half-plane. In terms of the dimensionless time $\tau = t/T = \xi + i\eta$, they are given by

$$\tau_k^\pm = \pm \xi_k + i\eta_k, \quad (30a)$$

$$\xi_k = \frac{1}{2} \sqrt{4(\ln \alpha)^2 + (2k+1)^2 \pi^2 + 2 \ln \alpha}, \quad (30b)$$

$$\eta_k = \frac{1}{2} \sqrt{4(\ln \alpha)^2 + (2k+1)^2 \pi^2 - 2 \ln \alpha}, \quad (30c)$$

where $k = 0, 1, 2, \dots$ and

$$\alpha = \frac{\sqrt{\pi}}{T \Omega_0}. \quad (31)$$

For $\alpha \ll 1$, we have

$$\xi_k \sim \frac{(2k+1)\pi}{4\sqrt{\ln(1/\alpha)}}, \quad (\alpha \ll 1), \quad (32a)$$

$$\eta_k \sim \sqrt{\ln(1/\alpha)}, \quad (\alpha \ll 1). \quad (32b)$$

Hence, as α decreases, the transition points approach the imaginary axis and in the limit $\alpha \rightarrow 0$ coalesce (logarithmically) with their counterparts in the second quadrant.

As we have mentioned the transition probability for the models chosen to satisfy the DDP optimization condition (26) show oscillating behavior, although they should yield optimized adiabatic passage. This is due to the fact that DDP is approximate method. A particular model without transition points in the diabatic basis, generally has a transition point in the first adiabatic basis. As in the Gaussian model the contributions from this transition points lead to oscillations, according to DDP formula (19). It is important to note the relation between the asymptotic behaviour of the transition points for $\alpha \ll 1$ and the adiabatic limit. From the definition of the model (29) is clear that the limit $T \rightarrow \infty$ can be seen as the adiabatic limit, so $1/T$ play role of the adiabatic parameter. From the definition (31) we see that α is proportional to the adiabatic parameter and the limit $\alpha \rightarrow 0$ is the adiabatic limit. According to the asymptotic behavior of the transition points, the transition point from the first quadrant logarithmically coalesce with their counterpart in the second quadrant and approach the imaginary axis. Since in the limit $\alpha \rightarrow 0$, which is perfect adiabatic regime, we do not have a coherent contribution to the DDP formula (19) from two transition points, no oscillations will be seen. This simple analysis shows that even in the first adiabatic basis, the correct asymptotic behaviors of the optimized adiabatic passage is achieved.

2. DDP integrals

Because for the Gaussian model (??) there are infinitely many transition points, the most accurate transition probability is expected to be given by the generalized DDP formula (19). The dominant contributions to the sum in this formula originate from the two transition points closest to the real axis, τ_0^- and τ_0^+ . For simplicity, we neglect the contributions from all others and retain only the terms from these two points.

Because $(\tau_0^-)^* = -\tau_0^+$ and because $\mathcal{E}(\tau)$ is an even function of time, it is easy to show that

$$\mathcal{D}(\tau_0^-) = -\mathcal{D}^*(\tau_0^+), \quad (33)$$

that is $\text{Re}\mathcal{D}(\tau_0^-) = -\text{Re}\mathcal{D}(\tau_0^+)$ and $\text{Im}\mathcal{D}(\tau_0^-) = \text{Im}\mathcal{D}(\tau_0^+)$. Hence it is sufficient to calculate only one of these integrals and we choose $\mathcal{D}(\tau_0^+)$ for this purpose.

Because the imaginary part of the DDP integral $\mathcal{D}(\tau)$ is the same for the two transition points τ_0^+ and τ_0^-

[cf. Eq. (33)], these points lie on the same Stokes line, defined by Eq. (??). This Stokes line extends from $-\infty$ to $+\infty$, which is a necessary condition for the validity of the DDP approximation [8?].

With the arguments presented above, the problem is reduced to the calculation of the DDP integral

$$\mathcal{D}(\tau_0^+) = \Delta T \int_0^{\tau_0^+} \sqrt{\alpha^2 e^{-2\tau^2} + 1} d\tau. \quad (34)$$

The estimation of this integral will be our main concern hereafter in this section.

a. Asymptotic behavior of the DDP integral for small α For small α ($\alpha \ll 1$) we expand the integrand in Eq. (34) by using the Taylor expansion, and perform term-by-term integration. This integration is justified within the circle $|x| \leq 1$, where the series (??) is uniformly convergent. We choose the path of integration to be the straight line from $\tau = 0$ to $\tau = \tau_0^+$ and parameterize this path as $\tau = \tau_0^+ s$ ($0 \leq s \leq 1$). It is easy to see that $|\alpha^2 e^{-2\tau^2}| \leq 1$ along this path. Indeed,

$$|\alpha^2 e^{-2\tau^2}| = \alpha^2 |e^{-2(\tau_0^+)^2 s^2}| = \alpha^{2(1-s^2)} \leq 1,$$

because $\alpha < 1$ and $0 \leq s \leq 1$.

By using the relation

$$\int_0^{\tau_0^+} e^{-2nu^2} du = \frac{\sqrt{\pi} \text{Erf}(\tau_0^+ \sqrt{2n})}{2\sqrt{2n}}, \quad (35)$$

we find that

$$\begin{aligned} \mathcal{D}(\tau_0^+) = \Delta T & \left[\tau_0^+ + \sum_{n=1}^{\infty} (-1)^{n-1} \frac{(2n-3)!!}{(2n)!!} \right. \\ & \times \left. \frac{\alpha^{2n} \sqrt{\pi} \text{Erf}(\tau_0^+ \sqrt{2n})}{2\sqrt{2n}} \right], \end{aligned} \quad (36)$$

3. Uniform approximation to the DDP integral

It is shown in [?] , one can derive a uniform approximation to the DDP integral $\mathcal{D}(\tau_0^+)$, Eq. (34), by choosing an appropriate integration contour.

a. Imaginary part of the DDP integral For the imaginary part of the DDP integral (34) we have

$$\text{Im}\mathcal{D}(\tau_0^+) \approx \frac{1}{2} \Delta T \sqrt{\sqrt{4 \ln^2(m\alpha) + \pi^2} - 2 \ln(m\alpha)}. \quad (37)$$

and $m \approx 1.311468$.

The advantage of this choice is that the approximation (37), besides providing the exact result for $\alpha = 1$ is also very accurate in some vicinity of this important point. On the other hand, Eq. (37) has the following asymptotics

$$\text{Im}\mathcal{D}(\tau_0^+) \sim \Delta T \sqrt{\ln(m/\alpha)}, \quad (\alpha \ll 1), \quad (38a)$$

These expressions agree with Eqs. (??) and (??), except for the factor m , which is insignificant in the limits $\alpha \gg 1$ and $\alpha \ll 1$ [since $\ln(m\alpha) = \ln m + \ln \alpha \approx \ln \alpha$ for $\alpha \gg 1$ and similarly for $\alpha \ll 1$]. This factor becomes significant for intermediate α , where, however, the accuracy of Eq. (37) improves until, as explained above, it becomes exact for $\alpha = 1$.

b. Real part of the DDP integral For the real part of the DDP integral (34) we have

$$\text{Re}\mathcal{D}(\tau_0^+) = \Delta T [\mathcal{I}_1(\alpha) + \mathcal{I}_2(\alpha)]. \quad (39)$$

The integral $\mathcal{I}_1(\alpha)$ is approximated as

$$\mathcal{I}_1(\alpha) \approx \left(\sqrt{\alpha^2 + 1} - 1 \right) \sqrt{\frac{1}{2} \ln \frac{\alpha^2}{[1 + \nu (\sqrt{\alpha^2 + 1} - 1)]^2 - 1}}. \quad (40)$$

and $\nu = 0.462350...$ The second integral $\mathcal{I}_2(\alpha)$ is approximated as

$$\mathcal{I}_2(\alpha) \approx \frac{1}{2} \sqrt{\left[\ln \frac{\alpha^2}{\mu(2-\mu)} \right]^2 + \pi^2 + \ln \frac{\alpha^2}{\mu(2-\mu)}}, \quad (41)$$

where $\mu = 0.316193...$, and $\mu(2-\mu) = 0.532408...$

4. Transition probability

In order to sum the contributions from various DDP integrals we need the factors Γ_k , Eq. (20). One finds after simple algebra that

$$\Gamma(\tau_k^\pm) = \pm (-1)^k. \quad (42)$$

Collecting the results we find

$$\mathcal{P} \sim 4 \exp[-2\text{Im}\mathcal{D}(\tau_0^+)] \sin^2[\text{Re}\mathcal{D}(\tau_0^+)]. \quad (43)$$

In [?] , is shown that including the contributions from all transition points one can verify the following expression for the transition probability

$$\mathcal{P} \sim \frac{\sin^2[\text{Re}\mathcal{D}(\tau_0^+)]}{\cosh^2[\text{Im}\mathcal{D}(\tau_0^+)]}. \quad (44)$$

Equation (44) provides a very accurate description of the transition probability \mathcal{P} . This approximation is plotted on Fig. 1 as a function of the peak Rabi frequency Ω_0 for four different values of the detuning Δ . As Ω_0 increases, Rabi-like oscillations are observed, with both amplitude and frequency matched very well by our approximation (44).

B. Deviation from optimized pulses

The DDP based approximation for the transition probability can be derived in the case of absent transition

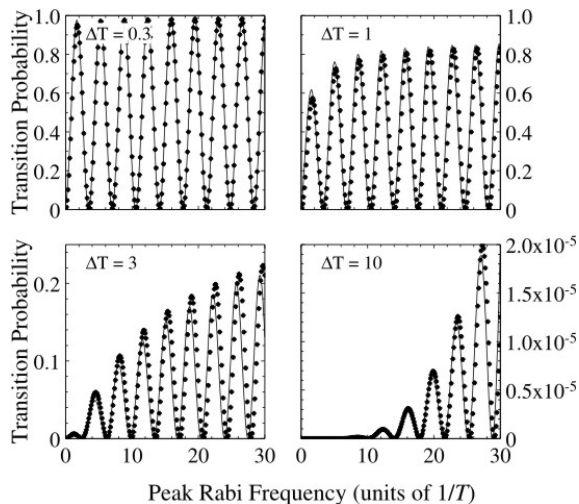


FIG. 1: Transition probability for the Gaussian pulse plotted vs the peak Rabi frequency Ω_0 for four values of the detuning, $\Delta T = 0.3, 1, 3, 10$. The exact results obtained by numerical integration of the Schrödinger equation are shown by dots and the approximation by solid lines.

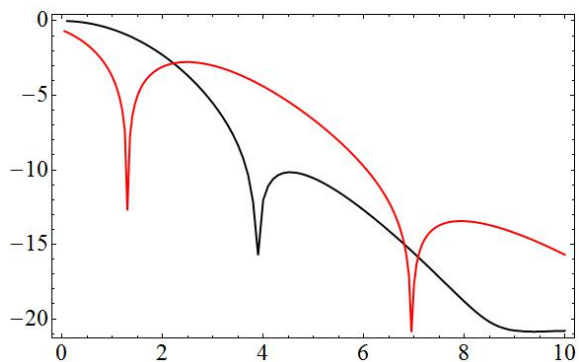


FIG. 2: $\ln(1 - \mathcal{P})$ as a function of Rabi frequency Ω_0 . Black curve shows the pulses given in Eq.(29), Red curve shows pulses given with Eq.(45) for $\mu = 1$

points by using the same DDP technique but in the first adiabatic basis. A very reasonable question is how we can derived transition probability whenever a small deviation from optimized pulses takes place. Instead of the optimized pulses given by Eq.(29) we introduce

$$\Delta(t) = (\Omega_0 + \mu) \sin \left[\frac{\pi}{2} \text{erf}(t/T) \right], \quad \Omega(t) = \Omega_0 \cos \left[\frac{\pi}{2} \text{erf}(t/T) \right] \quad (45)$$

where μ stands for small parameter. If we apply DDP for such model, for $\mu = 0$ as have been shown DDP fails to describe transition probability. This is true not only for $\mu = 0$ but for some vicinity of this point.

Figure 2 displays in Log scale $1 - \text{transition probability } \mathcal{P}$ i.e. $\ln(1 - \mathcal{P})$ for the adiabatic optimized pulses given in Eq.(29) and pulses given with Eq.(45) as a function of peak Rabi frequency Ω_0 .

IV. CONCLUSIONS

We have examined the optimization via DDP method in the superadiabatic basis. According to the DDP method models that do not have transition points would lead to vanishing nonadiabatic corrections. This would be the essence of the optimization based on DDP technique. We have shown that this condition is not sufficient for perfect adiabatic optimization. This is due to the approximate origin of the DDP method itself. Nevertheless DDP has been derived in order to take into account higher order adiabatic corrections, even for models that should yield according to DDP perfect adiabatic evolution (i.e. there are no transition points) within the the next adiabatic basis consecutive optimization is possible.

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